

Numerical study of the Transverse Diffusion coefficient for a one component model of a plasma

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We report the results of MD numerical simulations for a one component model of a plasma in the weakly coupled regime, at different values of temperature T and applied magnetic field \vec{B} , in which the diffusion coefficient D_{\perp} transverse to the field is estimated. We find that there exists a threshold in temperature, at which an inversion occurs, namely, for T above the threshold the diffusion coefficient D_{\perp} starts decreasing as T increases. This is at variance with the behavior predicted by the Bohm law $D_{\perp} \sim T/B$, which actually holds below the threshold. In addition we find that, for temperatures above such a threshold, another transition occurs, now with respect to the values of the magnetic field: for weak magnetic fields the diffusion coefficients scales as $1/B^2$, in agreement with the predictions of the standard kinetics theory, while it apparently saturates when the field strength is sufficiently increased.

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In this letter we report the results of some Molecular Dynamics simulations of a one component model of plasma. In particular we estimate the diffusion coefficient D_{\perp} transverse to the magnetic field, in the case of a weakly coupled plasma, for different values of temperature T and of magnetic field strength B .

Up to now, Molecular Dynamics simulations for the diffusion coefficient were implemented only for the case of strongly coupled plasmas, see for example the recent paper [1]. The general conclusion of that paper can be summarized by saying that, in the strongly coupled case, the diffusion coefficient obeys the scaling law $D_{\perp} \propto TB^{-1}$ proposed long ago by Bohm (see Table 1, page 135003-2 of [1]).

Our computations, while confirming the ones of paper [1] for the strongly coupled case, indicate that some important differences arise in the weakly coupled regime. In particular there exists a threshold in the coupling parameter, such that

- concerning the dependence on T , at variance with Bohm's law, above the threshold the diffusion coefficient D_{\perp} starts decreasing as temperature increases;
- concerning the dependence on B , one finds that D_{\perp} decreases as B^{-2} for small fields, but then apparently saturates to a constant value for larger values of B .

The results of our computations are summarized in figure 1, where, in logarithmic scale, the value of the coefficient D_{\perp} is reported (full circles) as a function of the

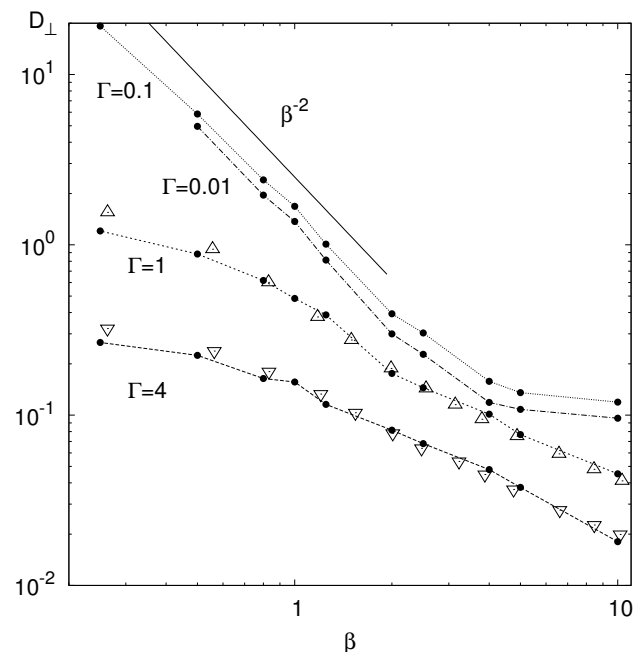


Figure 1: Diffusion coefficient transverse to the magnetic field versus β , as computed by MD simulations. Full circles are the results of our computations, while the empty triangles are values taken from paper [1]. The straight line corresponding to β^{-2} is also shown (dashed line).

dimensionless parameter β , defined by $\beta = B/\sqrt{nmc^2}$, where m is the electron mass, n the electron density and c the speed of light (we are working in the c.g.s. system). The different lines connect simulations performed at the same value of Γ , the dimensionless coupling parameter defined by $\Gamma = n^{1/3}e^2/(k_B T)$, where k_B is the

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Boltzmann constant, and e the electron charge. Such parameter discriminates between the strongly coupled case, corresponding to $\Gamma > 1$, and the weakly coupled case corresponding to $\Gamma \ll 1$.

For comparison, in the same figure are reported also some values (empty triangles) taken from reference [1], for Γ equal to 1.24 and 3.1 (corresponding to the values 2 and 5 if one uses the definition of Γ given in that paper). The agreement with our data seems to be good.

The figure clearly exhibits that, while for large values of Γ , actually up to 0.1, the coefficient D_\perp decreases as a function of Γ (i.e. is an **increasing** function of T), for the smaller value $\Gamma = 0.01$ an inversion occurs, i.e. the values of D_\perp are **smaller** than the corresponding values at $\Gamma = 0.1$. So there must exist a threshold in Γ , below which D_\perp becomes a **decreasing** function of T .

A straight line corresponding to β^{-2} is also shown. One can check that up to $\beta = 1$, the data for $\Gamma = 0.1$ and $\Gamma = 0.01$ seem to lie parallel to such a line. This means that, at fixed density, the coefficient D_\perp decreases as B^{-2} , as predicted by kinetic theory (see [2, 3]). However, by further increasing the magnetic field above $\beta = 1$, the diffusion coefficient appears to saturate to an apparently constant value independent of B . To our knowledge, this phenomenon was neither observed nor foreseen before.

The only reported evidence of some kind of transition that should occur in a weakly coupled plasma, when passing from $\beta \lesssim 1$ (weakly magnetized) to $\beta \gtrsim 1$ (strongly magnetized) was given in [4]. In that paper, such a transition was ascribed to a transition from a fully chaotic regime (low magnetic field) to a partially ordered one (high magnetic field), as first proposed in paper [5].

We now illustrate how a change of the dynamical behavior, might also explain the behavior of D_\perp reported above. We recall (see for example the textbook [6]) that the diffusion coefficient can be expressed in terms of the velocity autocorrelation $\langle \vec{v}_\perp(t) \cdot \vec{v}_\perp(0) \rangle$ as follows

$$D_\perp = \frac{1}{2} \int_0^{+\infty} \langle \vec{v}_\perp(t) \cdot \vec{v}_\perp(0) \rangle dt, \quad (1)$$

where \vec{v}_\perp is the component of the velocity of a particle, transverse to the magnetic field, and the brackets mean a suitable average over the particles. Now, in figure 2 we report the velocity spectrum, i.e. the Fourier transform of the autocorrelation, calculated at $\Gamma = 0.1$, for two values of β (below and above $\beta = 1$). One sees that in both cases, a strong peak occurs at the corresponding cyclotron frequency $\omega_c := eB/mc$, so that one can suppose that

$$\langle \vec{v}_\perp(t) \cdot \vec{v}_\perp(0) \rangle \simeq \langle \vec{v}_\perp(0) \cdot \vec{v}_\perp(0) \rangle \cos(\omega_c t) f(t),$$

where $f(t)$ is a function which characterizes the decay to zero of the autocorrelation as $t \rightarrow +\infty$. In the fully chaotic regime one can take $f(t) = e^{-\gamma t}$, where γ is the inverse of the decorrelation time. If such a time is larger than the cyclotron period, from eq. (1) one gets

$$D_\perp = \frac{k_B T}{m} \frac{\gamma}{\omega_c^2}. \quad (2)$$

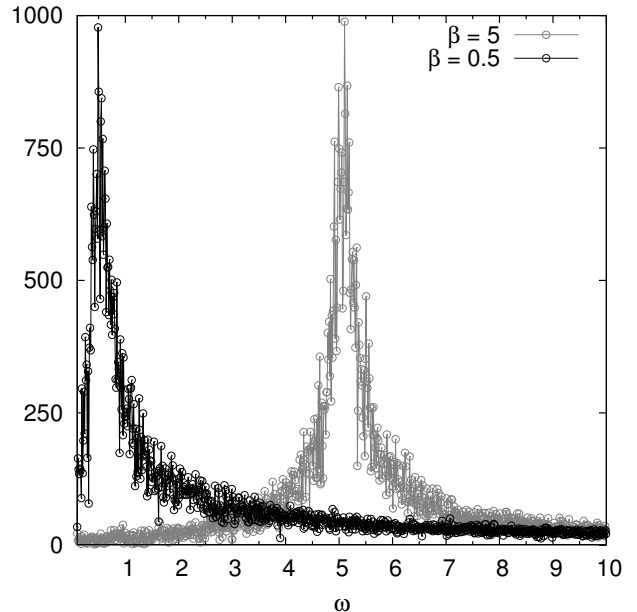


Figure 2: Fourier transform of the velocity autocorrelation function $\langle \vec{v}_\perp(t) \cdot \vec{v}_\perp(0) \rangle$, obtained in two simulations, with the same value $\Gamma = 0.1$, and two different values of β , namely, $\beta = 0.5$ (black line) and $\beta = 5$. (gray line). The frequencies are reported in units of ω_p . Notice the peaks centered at the corresponding cyclotron frequencies.

This expression shows that D_\perp decreases as B^{-2} , in agreement with our numerical data for small B .

Instead one can suppose that, in a partially ordered case, the decay of correlations is much slower, for example as an inverse power of time. Taking for example $f(t) = 1/(1 + (\gamma^* t)^2)$, one gets the expression

$$D_\perp = \frac{k_B T}{m} \frac{\pi}{2} \frac{\exp(-\omega_c/\gamma^*)}{\gamma^*}. \quad (3)$$

Now one needs to match the expression (2) with (3) at ω_c equal to the plasma frequency $\omega_p := \sqrt{e^2/n}$, i.e., for $\beta = 1$, which is precisely the value of the threshold predicted in reference [5]. Given a value of γ/ω_p , this matching determines two possible values of γ^*/ω_p , one smaller than 1 and one bigger. If one chooses the larger one, the expression (3) for $\omega_c \simeq \omega_p$ gives a curve with a slope much smaller than the curve (2), thus reproducing the behavior found numerically. At very large values of ω_c , the diffusion coefficient D_\perp should begin to decrease faster than any inverse power of B , but this range is actually outside our reach. At any rate, a decrease of D_\perp faster than any inverse power of B , is reported in reference [7], and could actually be ascribed to the phenomenon just described.

We give now some details of our numerical computations. First of all, for the purpose of estimating D_\perp , it is better to use directly its definition, instead of making

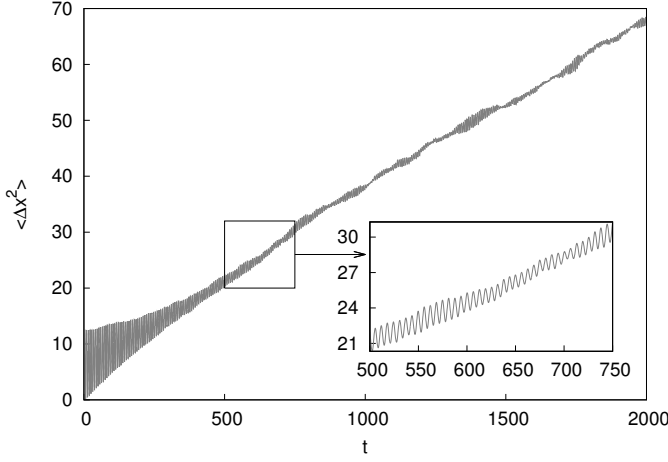


Figure 3: Graph of $\langle |\Delta \vec{x}_\perp|^2 \rangle$ vs time t (in ω_c^{-1} units) in the case $\Gamma = 0.01$ and $\beta = 4$.

use of relation (1). We recall that the transverse diffusion coefficient is defined by

$$D_\perp = \lim_{t \rightarrow \infty} \frac{\langle |\Delta \vec{x}_\perp|^2 \rangle}{4t} \quad (4)$$

where

$$|\Delta \vec{x}_\perp|^2 := |x(t) - x(t_0)|^2 + |y(t) - y(t_0)|^2, \quad (5)$$

i.e., as the mean square displacement of a particle in the plane orthogonal to the magnetic field \vec{B} (which is taken directed as the z -axis) and the average should in principle be an average over all the plasma particles. The quantity in eq. (4) can be computed from a numerical simulation by averaging over the particles which participate to the simulation, while the asymptotic value can be found from the plot of $\langle |\Delta \vec{x}_\perp|^2 \rangle$ versus t . A typical example of such a plot is shown in Fig. 3; as one can see, it displays an oscillatory behavior superimposed to a linear growth, and a ballistic motion at the beginning. To remove the oscillations we replaced each value of $\langle |\Delta \vec{x}_\perp|^2 \rangle(t)$ by its mean value $\bar{X}(t)$ taken over a cyclotron period centered at t . The resulting data were analyzed with a linear regression of the law $\bar{X} = Dt + C$, with two constants C and D . Here one has to choose a temporal window to include only the tail of the graph; we progressively restricted such window until the reduced error χ (the sum of the squared residual divided by the number of points minus 2) became less than 1. The values thus found are reported in figure 1.

For what concerns the model, we recall that the one component model of a plasma consists of a gas of electrons moving in a fixed uniform neutralizing background. So we consider a number N of electrons in a cubic box of side L with periodic boundary conditions, the electrons being subject to mutual Coulomb interactions, and to an external magnetic field $\vec{B} = B\vec{e}_z$. The density is then defined by $n = N/L^3$.

If t denotes time and \vec{x}_i the position of the i -th electron (with $i = 1, \dots, N$), with the rescaling

$$\vec{y}_i = n^{-1/3} \vec{x}_i, \quad \tau = \omega_c t, \quad m = 1, \quad (6)$$

which in particular implies that the density takes the value 1, the equations of motion read

$$\frac{d^2 \vec{y}_i}{d\tau^2} = \vec{e}_z \times \frac{d\vec{y}_i}{d\tau} + \frac{1}{\beta^2} \sum_{j \neq i} \vec{E}_j(\vec{y}_i) \quad (7)$$

where \vec{E}_j is the electric field created by the j -th electron, evaluated at the position of the i -th one. The total electric field $\vec{E} = \sum_{j \neq i} \vec{E}_j$ acting on an electron, created by a periodic system of charges, can be computed via the Ewald formula (see [8]), as follows

$$\begin{aligned} \vec{E}(\vec{y}_i) = & \sum_{\vec{l}} \sum_{j=1}^N \frac{\vec{y}_{ij\vec{l}}}{|\vec{y}_{ij\vec{l}}|^3} \left[\text{erfc}(\alpha |\vec{y}_{ij\vec{l}}|) + \frac{2\alpha |\vec{y}_{ij\vec{l}}|}{\sqrt{\pi}} \exp(-\alpha^2 |\vec{y}_{ij\vec{l}}|^2) \right] \\ & + \frac{4\pi}{N} \sum_{\vec{k} \neq 0} \sum_{j=1}^N \frac{\vec{k}}{k^2} e^{-k^2/4\alpha^2} \sin(\vec{k} \cdot \vec{y}_{ji}), \quad \alpha = \frac{\sqrt{\pi} N^{1/6}}{L} \end{aligned}$$

Here $\vec{y}_{ij\vec{l}} = \vec{y}_i - \vec{y}_j + \vec{l}$, where \vec{l} is a triplet of integers denoting the position of an image cell. One has to point out that only the parameter β enters into the equations of motion. The second one Γ , enters through the choice of the initial data: indeed, while the positions are extracted from a uniform distribution, the velocities are taken from a Maxwell distribution at temperature T . With this choice, at the beginning of each simulation the system is out of equilibrium: so there is a drift of the kinetic energy, and the system reaches a different, random, temperature. In order to fix the temperature to the desired value, we operate in this way: after extracting the initial values, we let the system evolve until equilibrium is reached, i.e. until the kinetic energy appears to stabilize. We then generate new velocities again with a Maxwell distribution at temperature T , and repeat the process until the kinetic energy appears to be constant, close to the chosen value.

Equations (7) are integrated using a symplectic splitting algorithm. The inter particle forces are computed with the aid of parallel calculators, using GPUs with up to 15 multiprocessors. But even with such a device, we cannot afford to integrate the equations of motion for small values of Γ , and we have to stop at $\Gamma = 0.01$. This for two problems which arise in the weakly coupled regime.

The first problem concerns the integration step h . In fact, as the velocities are proportional to $\Gamma^{-1/2}$, to achieve a good energy conservation when short distance collisions occur, one has to use a very small time step. A step $h = 10^{-3}$ is sufficiently small for the strongly coupled cases, in which conservation of energy was always better than 0.05%. The step had to be reduced up to

$h = 2.5 \times 10^{-5}$ for $\Gamma = 0.01$. Curiously enough, it seems that also the value of β has an influence on the choice of h . For example, if $\beta = 10$, the value $h = 10^{-3}$ proved to be adequate even in the case $\Gamma = 0.01$. The error on conservation of energy is still below 0.05% for $\Gamma = 0.1$ but increases up to 0.5% for $\Gamma = 0.01$.

The second problem is that, working with periodic boundary conditions, one should have the fundamental cell with side larger than the Debye length λ_D , which in our units reads $\lambda_D = \sqrt{1/\Gamma}$. As in the rescaled variables the density has value 1, we have $L = N^{1/3}$, so that the requirement $L > \lambda_D$ in our units takes the form of the constraint $N > \Gamma^{-3/2}$, which is a very stringent condition in the weakly coupled regime $\Gamma \ll 1$. Indeed, as the Coulomb force is a long range one, the computational cost increases as N^2 , i.e., increases as Γ^{-3} . This means that the computational cost increases at least a thousand times by decreasing Γ by a factor ten. Actually, as one must also decrease the value of the integration step, the computational cost increases even more. Now, although

in the strongly coupled cases a single particle would satisfy the constraint, we actually used 480 particles. In the cases $\Gamma = 0.1$ and 0.01 instead, for which the constraint gives $N > 31$ and $N > 1000$ respectively, we took $N = 896$ and $N = 1024$ respectively. This last figure is the maximum number of particles we can deal with. Computations with this number of particles take months to be completed.

Our data are affected by some fluctuations, due to various factors; mainly, we suppose, the very limited number of particles. In paper [1], in which a model essentially equal to ours was integrated, the authors report that a certain stability of the numerical results is obtained using a number of particles equal to $N = 8192$, which is beyond our reach. So this work should be intended, also numerically, as a preliminary one. Naturally, the main improvement would be to be able to simulate a two-component model, which however is, at the moment, far from our numerical capabilities.

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